Refined comparison theorems for the Dirac equation in d dimensions.

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A single spin-$^1/_2$ particle obeys the Dirac equation in $d \geq 1$ spatial dimension and is bound by an attractive central monotone potential which vanishes at infinity (in one dimension the potential is even). This work refines the relativistic comparison theorems which were derived by Hall [1]. The new theorems allow the graphs of the two comparison potentials V_a and V_b to crossover in a controlled way and still imply the spectral ordering $E_a \leq E_b$ for the eigenvalues at the bottom of each angular momentum subspace. More specifically in a simplest case we have: in dimension $d = 1$, if $\int_0^x (V_b(t) - V_a(t))dt \geq 0$, $x \in [0, \infty)$, then $E_a \leq E_b$; and in $d > 1$ dimensions, if $\int_0^r (V_b(t) - V_a(t))t^{2|k_d|}dt \geq 0$, $r \in [0, \infty)$, where $k_d = \tau \left(j + \frac{d-2}{2}\right)$ and $\tau = \pm 1$, then $E_a \leq E_b$.

I. INTRODUCTION

The comparison theorem of quantum mechanics states that if two comparison potentials are ordered, i.e. $V_a \leq V_b$, then the discrete energy eigenvalues are ordered as well $E_a \leq E_b$. In the nonrelativistic case this is a straightforward consequence of the min–max variational characterization of the discrete part of the spectrum [2, 3]. In the relativistic case the Hamiltonian is not bounded below, and a variational analysis is more complicated [4–6]. However, comparison theorems have been established by other means in $d = 1$ and $d = 3$ dimensions [1], in $d = 2$ dimensions [7], and in d dimensions [8], most recently by monotonicity arguments [9–12]. In Ref. [13] Semay used the Hellmann–Feynman theorem [14] to established a general comparison theorem for the Schrödinger and Dirac equations.

In this paper we derive *refined* comparison theorems which allow the graphs of the comparison potentials to cross over in a controlled fashion and still imply definite ordering of the respective eigenvalues at the bottom of each angular-momentum subspace. This idea was first explored by Hall *et al* for nonrelativistic problems in $d = 1$ and $d = 3$ dimensions [15] and in $d > 1$ dimensions [16], and applied to Sturm–Liouville problems in [17]. In the simplest case one derives the spectral ordering $E_a \leq E_b$ from the weaker potential assumption $U_a \leq U_b$, where $U_i = \int_0^x V_i(t)dt$, $i = a$ or b. Since these refined nonrelativistic results were obtained *without* the use of a variational characterization of the discrete spectrum, similar reasoning could be applied to derive a basic relativistic comparison theorem for the Dirac equation [1]. The principal aim of the present paper is to go further and derive refined comparison theorems also for the Dirac spectral problem itself.

In dimension $d = 1$, the energies compared are simply the lowest discrete eigenvalues. In $d > 1$ dimensions, the energies are the lowest eigenvalues in each angular-momentum sector. The derivations rely on *a priori* knowledge of the nodal structure characterized for central fields in Refs. [18–20]. We found it necessary to discuss the cases $d = 1$ and $d > 1$ separately and to treat a small number of distinct classes of attractive monotone potentials. Sharper energy bounds can be obtained if the component wave functions are also known for the chosen base comparison potential. Simple sufficient conditions are derived in corollaries to the comparison theorems to make their use more immediate and straightforward. The results are illustrated by some specific examples.

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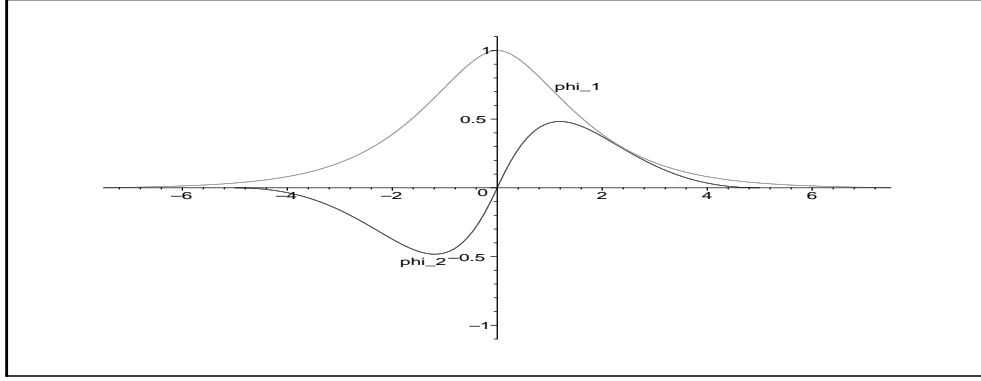†Electronic address: petrzorin@yahoo.com

FIG. 1: Ground state wave functions φ_1 and φ_2, corresponding to the exponential potential $V = -\beta e^{-b|x|}$, with $\beta = 0.9$, $b = 0.5$, $m = 1$, and energy is $E = 0.49233$.

II. DIRAC EQUATION IN ONE DIMENSION

The Dirac equation in one spatial dimension for a single spin-$1/2$ particle of mass m in natural units $\hbar = c = 1$ may be written [21]:

$$\left(\sigma_1 \frac{\partial}{\partial x} - (E - V)\sigma_3 + m \right) \psi = 0,$$

where σ_1 and σ_3 are Pauli matrices and the discrete energy eigenvalue E such that $-m < E < m$, [22, 23]. The vector potential V (the time component of a four–vector) satisfies

(i) V is even, i.e. $V(x) = V(-x)$;

(ii) V is nonpositive and bounded, i.e. $V_0 \leq V \leq 0$, where $V_0 = V(0)$;

(iii) V vanishes at infinity, thus $\lim\limits_{x \to \pm\infty} V = 0$;

(iv) V is attractive, that is monotone nondecreasing on $[0, \infty)$.

By taking the two–component Dirac spinor as $\psi = \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix}$ the above matrix equation can be decomposed into a system of first–order linear differential equations [24, 25]:

$$\begin{cases} \varphi_1' = -(E + m - V)\varphi_2, & \text{(1a)} \\ \varphi_2' = \ \ (E - m - V)\varphi_1, & \text{(1b)} \end{cases}$$

where prime $'$ denotes the derivative with respect to x. For bound states, φ_1 and φ_2 satisfy the normalization condition

$$(\varphi_1, \varphi_1) + (\varphi_2, \varphi_2) = \int\limits_{-\infty}^{\infty} (\varphi_1^2 + \varphi_2^2)dx = 1.$$

For the reason which will be clear later, the comparison theorem below requires knowledge concerning the ground state. According to the Nodal Theorem of Ref.[20], the upper and lower components of the Dirac spinor, φ_1 and φ_2 respectively, have definite and opposite parities and $n_2 = n_1 + 1$, where n_i, $i = 1$ or 2, the corresponding number of nodes of φ_i. Thus in the state with the smallest number of nodes, the upper component φ_1 is even and the lower one φ_2 is odd. From now on, without loss of generality, we consider the interval $[0, \infty)$ and assume that both components of the Dirac spinor lie above the x–axis, i.e. $\varphi_1 \geq 0$ and $\varphi_2 \geq 0$ on $[0, \infty)$. Then it follows from (1a)–(1b) that on $[0, \infty)$, $\varphi_1' \leq 0$ and $\varphi_2' \geq 0$ near the origin then $\varphi_2' \leq 0$ at infinity. As an illustration we plot $\{\varphi_1, \varphi_2\}$ for the exponential potential $V = -\beta e^{-b|x|}$ [26] (see Figure 1).

III.   REFINED COMPARISON THEOREMS FOR THE DIRAC EQUATION IN ONE DIMENSION

We compare two problems with symmetric potentials V_a and V_b and ground state energies E_a and E_b for which the system (1a)–(1b) becomes respectively

$$\begin{cases} \varphi'_{1a} = -(E_a + m - V_a)\varphi_{2a}, & \text{(2a)} \\ \varphi'_{2a} = (E_a - m - V_a)\varphi_{1a}, & \text{(2b)} \end{cases}$$

and

$$\begin{cases} \varphi'_{1b} = -(E_b + m - V_b)\varphi_{2b}, & \text{(3a)} \\ \varphi'_{2b} = (E_b - m - V_b)\varphi_{1b}. & \text{(3b)} \end{cases}$$

Let us consider the combination of equations:

$$(2a)\varphi_{2b} - (2b)\varphi_{1b} - (3a)\varphi_{2a} + (3b)\varphi_{1a}, \tag{4}$$

which after some simplifications becomes

$$(\varphi_{1a}\varphi_{2b})' - (\varphi_{2a}\varphi_{1b})' = (\varphi_{1a}\varphi_{1b} + \varphi_{2a}\varphi_{2b})\left[(E_b - E_a) - (V_b - V_a)\right].$$

Integrating the left side of the above expression by parts from 0 to ∞ and using the boundary conditions, $\varphi_{1a}(0) = \varphi_{1b}(0) = 0$ and $\lim_{x \to \infty} \varphi_{2a} = \lim_{x \to \infty} \varphi_{2b} = 0$, we find $\int_0^\infty \left[(\varphi_{1a}\varphi_{2b})' - (\varphi_{2a}\varphi_{1b})'\right] dx = 0$. Then we integrate the right side to obtain

$$(E_b - E_a)\int_0^\infty (\varphi_{1a}\varphi_{1b} + \varphi_{2a}\varphi_{2b})dx = \int_0^\infty (\varphi_{1a}\varphi_{1b} + \varphi_{2a}\varphi_{2b})(V_b - V_a)dx. \tag{5}$$

It follows from the last expression that if the wave functions have no nodes, so that the integrands have constant signs, and the potentials are ordered i.e. $V_a \leq V_b$, then $E_a \leq E_b$. This is the comparison theorem which was first proved in $d = 3$ dimensions in [1], in $d = 2$ dimensions in [7], and in d dimensions in [8]. Later, using the monotonicity concept, the comparison theorem was proved for higher dimension cases $d \geq 1$ for the Dirac equation in [11] and the Klein–Gordon equation in [12] for all the excited states.

The Dirac equation admits exact analytical solutions for very few potentials. The above theorem allows us to obtain upper or lower bounds for any eigenvalue with the aid of suitable comparison potentials. But the comparison potentials can not cross each other, because in that case the integrands of (5) change sign. Similarly to the nonrelativistic case [15] we now derive refined relativistic comparison theorems which allow the graphs of the potentials to crossover in a controlled manner so that spectral ordering is predicted.

Theorem 1:   *The potential V satisfies (i)–(iii), $-V_0 \leq 2m$, and has area. Then if*

$$g(x) = \int_0^x (V_b(t) - V_a(t))dt \geq 0, \quad x \in [0, \infty), \tag{6}$$

we have $E_a \leq E_b$.

Proof: We integrate the right side of (5) by parts to obtain

$$\int_0^\infty (\varphi_{1a}\varphi_{1b} + \varphi_{2a}\varphi_{2b})(V_b - V_a)dx = (\varphi_{1a}\varphi_{1b} + \varphi_{2a}\varphi_{2b})g|_0^\infty - \int_0^\infty g(\varphi_{1a}\varphi_{1b} + \varphi_{2a}\varphi_{2b})'dx,$$

where $g(x)$ is defined by (6). Since $g(0) = 0$ and $\lim_{x \to \infty} \varphi_{1a} = \lim_{x \to \infty} \varphi_{2a} = 0$, relation (5) becomes

$$(E_b - E_a)\int_0^\infty (\varphi_{1a}\varphi_{1b} + \varphi_{2a}\varphi_{2b})dx = -\int_0^\infty g(\varphi_{1a}\varphi_{1b} + \varphi_{2a}\varphi_{2b})'dx. \tag{7}$$

In order to find the sign of $(\varphi_{1a}\varphi_{1b} + \varphi_{2a}\varphi_{2b})'$ we write

$$(\varphi_{1a}\varphi_{1b} + \varphi_{2a}\varphi_{2b})' = W_1\varphi_{1b}\varphi_{2a} + W_2\varphi_{1a}\varphi_{2b},$$

where

$$W_1 = -E_a + E_b - 2m + V_a - V_b \quad \text{and} \quad W_2 = E_a - E_b - 2m - V_a + V_b.$$

Let φ_2 represent either φ_{2a} or φ_{2b}. Suppose that φ_2 reaches its maximum at some point x_c; thus $\varphi_2' \geq 0$ on $[0, x_c]$ and $\varphi_2' \leq 0$ on $[x_c, \infty)$. It follows from (1b) that $E_a - m - V_a \geq 0$ on $[0, x_c]$, so $W_1 < E_b - V_b - 3m$. Since $-V_b \leq 2m$ and $-m < E_b < m$, $W_1 < 0$ on $[0, x_c]$. Then on $[x_c, \infty)$ equation (1b) implies $E_b - m - V_b \leq 0$, which leads to $W_1 \leq -E_a - m + V_a$, energy E_a satisfies $-m < E_a < m$ so $W_1 < 0$ on $[x_c, \infty)$. Therefore $W_1 < 0$ on $[0, \infty)$. Similarly it can be shown that $W_2 < 0$ on $[0, \infty)$. Thus $(\varphi_{1a}\varphi_{1b} + \varphi_{2a}\varphi_{2b})' \leq 0$, on $[0, \infty)$. Therefore if $g(x) \geq 0$ relation (7) ensures that $E_a \leq E_b$, which result completes the proof of the theorem.

$\square$

If we know the exact behaviour of the comparison potentials we can state simpler sufficient conditions for spectral ordering:

Corollary 1: *If the potentials cross over once, say at x_1, $V_a \leq V_b$ for $x \in [0, \ x_1]$, and*

$$g(\infty) = \int_0^\infty (V_b - V_a)dx \geq 0,$$

then $E_a \leq E_b$. If the potentials cross over twice, say at x_1 and x_2, $x_1 < x_2$, $V_a \leq V_b$ for $x \in [0, \ x_1]$, and

$$g(x_2) = \int_0^{x_2} (V_b - V_a)dx \geq 0,$$

then $E_a \leq E_b$.

We note that such application of Theorem 1 via the Corollary 1 can easily be extended. For example, consider the case of n intersections, $n = 1, \ 2, \ 3, \ \ldots$, and suppose again that $V_a \leq V_b$ for the first interval $x \in [0, \ x_1]$. Suppose now that the sequence $\int_{x_i}^{x_{i+1}} |V_b - V_a|dx$, $i = 1, \ 2, \ 3, \ \ldots, \ n$, of absolute areas is nonincreasing (if n is odd then $\int_{x_{n-1}}^{x_n} |V_b - V_a|dx \geq \int_{x_n}^\infty |V_b - V_a|dx$), consequently it follows that $\int_0^x (V_b(t) - V_a(t))dt \geq 0$, $x \in [0, \ \infty)$, and we conclude $E_a \leq E_b$.

Remark: we now also consider theorems which take advantage of the known wave functions for *one* of the two comparison potentials. The general concept here is that we use these known wave functions for one of the eigenproblems along with an assumed relationship between the two potentials, and from these conditions we predict bounds on the eigenvalues of the second problem. In each such theorem we choose the base comparison potential to be V_i where in an application i may be chosen to be either $i = a$ or $i = b$; of course, changing the base problem will also reverse the energy inequality from lower to upper bound, or *vice versa*. Now we state the second theorem (which allows the bottom of the potential to lie below $-2m$):

Theorem 2: *The potential V satisfies (i)–(iv) and has φ_{1i} and $t\varphi_{2i}$–weighted areas, if*

$$k_1(x) = \int_0^x (V_b(t) - V_a(t))\varphi_{1i}(t)dt \geq 0 \quad and \quad k_2(x) = \int_0^x (V_b(t) - V_a(t))\varphi_{2i}(t)tdt \geq 0, \quad x \in [0, \ \infty), \qquad (8)$$

where i is either a or b, then we have $E_a \leq E_b$.

Proof: We prove the theorem for $i = b$; for $i = a$, the proof is the same. We integrate the right side of (5) by parts to obtain

$$(E_b - E_a) \int_0^\infty (\varphi_{1a}\varphi_{1b} + \varphi_{2a}\varphi_{2b})dx = \left[k_1\varphi_{1a} + k_2 \frac{\varphi_{2a}}{x} \right]_0^\infty - \int_0^\infty \left[k_1\varphi_{1a}' + k_2 \left(\frac{\varphi_{2a}}{x} \right)' \right] dx,$$

where $k_1(x)$ and $k_2(x)$ are defined by (8) for $i = b$. The expression $\left[k_1\varphi_{1a} + k_2\frac{\varphi_{2a}}{x} \right]_0^\infty = 0$, because $k_1(0) = k_2(0) = 0$ and $\lim_{x \to \infty} \varphi_{1a} = \lim_{x \to \infty} \varphi_{2a} = 0$. The function φ_{1a} is positive and decreasing, thus $\varphi_{1a}' \leq 0$ on $[0, \infty)$. We know that $\varphi_{2a}' \geq 0$ on $[0, x_c]$ and $\varphi_{2a}' \leq 0$ on $[x_c, \infty)$. It follows that $(\varphi_{2a}/x)' \leq 0$ on $[x_c, \infty)$. From the assumption (iv) and (2b) we conclude $\varphi_{2a}'' \leq 0$, that is to say φ_{2a} is concave on $[0, x_c]$, so lies below its tangents lines: thus $\varphi_{2a}(x) \geq x\varphi_{2a}'(x)$, which implies $(\varphi_{2a}/x)' < 0$ on $[0, x_c]$. Therefore $(\varphi_{2a}/x)' \leq 0$ on $[0, \infty)$. Finally, if $k_1(x)$ and $k_2(x)$ are both nonnegative it follows from the above expression that $E_a \leq E_b$. This completes the proof.

$\square$

The second theorem is sronger because the potential difference $\triangle V = V_b - V_a$ is multiplied by the decreasing factor φ_{1i} in $k_1(x)$, and by $t\varphi_{2i}$ in $k_2(x)$, $i = a, \ b$, and this allows $\triangle V$ to be even larger than in Theorem 1 and still imply the spectral ordering $E_a \leq E_b$. Similarly to Corollary 1, but now with the φ_{ji}–weighted areas, $j = 1$ or 2 and $i = a$ or b, we can state the following sufficient condition for spectral ordering:
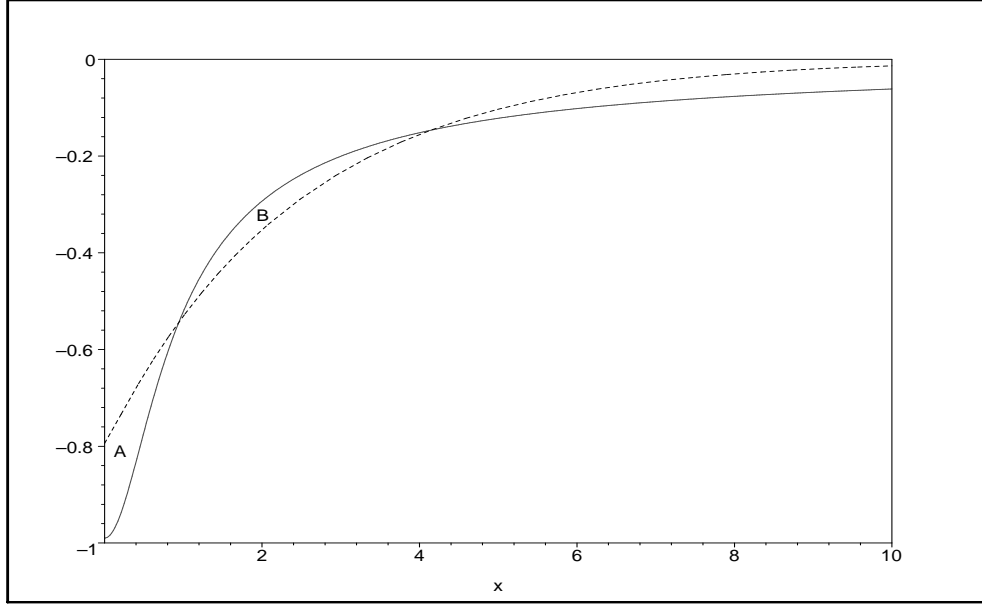
FIG. 2: The laser–dressed potential V_a full line and the exponential potential V_b dotted line.

Corollary 2: *If the potentials cross over once, say at x_1, $V_a \leq V_b$ for $x \in [0,\ x_1]$, and*

$$k_1(\infty) = \int_0^\infty (V_b - V_a)\varphi_{1i}dx \geq 0 \quad and \quad k_2(\infty) = \int_0^\infty (V_b - V_a)\varphi_{2i}xdx \geq 0, \quad i = a \ or \ b,$$

then $E_a \leq E_b$. If the potentials cross over twice, say at x_1 and x_2, $x_1 < x_2$, $V_a \leq V_b$ for $x \in [0,\ x_1]$, and

$$k_1(x_2) = \int_0^{x_2} (V_b - V_a)\varphi_{1i}dx \geq 0 \quad and \quad k_2(x_2) = \int_0^{x_2} (V_b - V_a)\varphi_{2i}xdx \geq 0, \quad i = a \ or \ b,$$

then $E_a \leq E_b$.

Corollary 2 can be generalized as well for the case of n intersections: if $V_a \leq V_b$ on $x \in [0,\ x_1]$ and the sequences $\int_{x_i}^{x_{i+1}} |V_b - V_a|\varphi_{1j}dx$ and $\int_{x_i}^{x_{i+1}} |V_b - V_a|\varphi_{2j}xdx$, $i = 1,\ 2,\ 3,\ \ldots,\ n$ and $j = a$ or b, of absolute areas are nonincreasing (and, if n is odd, $\int_{x_{n-1}}^{x_n} |V_b - V_a|\varphi_{1j}dx \geq \int_{x_n}^\infty |V_b - V_a|\varphi_{1j}dx$ and $\int_{x_{n-1}}^{x_n} |V_b - V_a|\varphi_{2j}xdx \geq \int_{x_n}^\infty |V_b - V_a|\varphi_{2j}xdx$), then $\int_0^x (V_b(t) - V_a(t))\varphi_{1j}(t)dt \geq 0$ and $\int_0^x (V_b(t) - V_a(t))\varphi_{2j}(t)tdt \geq 0$ on $x \in [0,\ \infty)$, so, according to Theorem 2, we conclude $E_a \leq E_b$.

An example

To demonstrate Theorem 1 we choose the laser–dressed potential V_a [27–29] and the exponential potential V_b in the form

$$V_a = -\frac{\alpha}{(x^2 + a^2)^{1/2}} \quad and \quad V_b = -\beta e^{-b|x|},$$

with $\alpha = 0.61362$, $a = 0.62$, $\beta = 0.8$, and $b = 0.41$; see Figure 2. Thus $V_a(0) = -0.989$ and $V_b(0) = -0.8$, and taking $m = 1$, the condition $-V_0 \leq 2m$ is satisfied. The graphs of V_a and V_b intersect at $x_1 = 0.94437$ and $x_2 = 4.13782$. Then we calculate areas A and B

$$A = \int_0^{x_1} (V_b - V_a)dx = 0.11456$$

and

$$B = \int_{x_1}^{x_2} (V_a - V_b)dx = 0.11455.$$

Since $A > B$ we have $g > 0$ therefore according to Corollary 1 we should have $E_a \leq E_b$, which we verify by calculating accurate numerical eigenvalues, i.e. $E_a = 0.45657 \leq E_b = 0.52332$.

IV.   DIRAC EQUATION IN $d > 1$ DIMENSIONS

For a central potential in $d > 1$ dimensions the Dirac equation can be written [30] in natural units $\hbar = c = 1$ as

$$i\frac{\partial \Psi}{\partial t} = H\Psi, \quad \text{where} \quad H = \sum_{s=1}^{d} \alpha_s p_s + m\beta + V,$$

where m is the mass of the particle, V is an attractive spherically–symmetric potential, which will be defined later, and $\{\alpha_s\}$ and β are Dirac matrices, which satisfy anti–commutation relations; the identity matrix is implied after the potential V. For stationary states, some algebraic calculations in a suitable basis, the details of which may be found in Refs. [31–35], lead to a pair of first–order linear differential equations in two radial wave functions $\{\psi_1, \psi_2\}$, namely

$$\begin{cases} \psi_1' = (m + E - V)\psi_2 - \dfrac{k_d}{r}\psi_1, & \text{(9a)} \\[2mm] \psi_2' = (m - E + V)\psi_1 + \dfrac{k_d}{r}\psi_2, & \text{(9b)} \end{cases}$$

where $r = \|\boldsymbol{r}\|$, prime $'$ denotes the derivative with respect to r, $k_d = \tau\left(j + \frac{d-2}{2}\right)$, $\tau = \pm 1$, and $j = 1/2,\ 3/2,\ 5/2,\ \ldots$. We note that the variable τ is sometimes written ω, as, for example in the book by Messiah [36], and the radial functions are often written $\psi_1 = G$ and $\psi_2 = F$, as in the book by Greiner [37]. For $d > 1$, these functions vanish at $r = 0$, and, for bound states, they may be normalized by the relation

$$(\psi_1, \psi_1) + (\psi_2, \psi_2) = \int_0^\infty (\psi_1^2 + \psi_2^2)dr = 1.$$

We use inner products *without* the radial measure $r^{(d-1)}$ because the factor $r^{\frac{(d-1)}{2}}$ is already built in to each radial function. We shall assume that the potential V is such that there is a discrete energy eigenvalue E and that equations (9a)–(9b) are the eigenequations for the corresponding radial eigenstates. Throughout this paper we will consider only potentials which vanish at infinity, thus the above system at infinity becomes

$$\begin{cases} \psi_1' = (m + E)\psi_2, & \text{(10a)} \\ \psi_2' = (m - E)\psi_1. & \text{(10b)} \end{cases}$$

Let us assume that $\psi_1 \geq 0$ before vainshing, then it follows from (10a) that $(m + E)\psi_2 \leq 0$. Thus either $m + E > 0$ and $\psi_2 \leq 0$ or $m + E < 0$ and $\psi_2 \geq 0$. By considering equation (10b), the first case leads to $\psi_2' \geq 0$ and $m - E > 0$, so $-m < E < m$. The second case leads to $\psi_2' \leq 0$ and $m - E < 0$; but this is the contradiction: it follows from $m + E < 0$ that $E < 0$ and from $m - E < 0$ that $E > 0$. Therefore we conclude that if the potential V vanishes at infinity then the discrete energy E is such that $-m < E < m$.

V.   REFINED COMPARISON THEOREMS FOR THE DIRAC EQUATION IN $d > 1$ DIMENSIONS

As in one–dimensional case we need to know some characteristics of the nodeless state of the Dirac coupled equations (9a)–(9b). It follows from the Nodal Theorem of Ref. [20] that in the state with no nodes $k_d < 0$, and either $\psi_1 \geq 0$ and $\psi_2 \leq 0$ or $\psi_1 \leq 0$ and $\psi_2 \geq 0$ for $r \in [0, \infty)$; so from now on without loss of generality we suppose $k_d < 0$ and $\psi_1 \geq 0$ and $\psi_2 \leq 0$ for $r \in [0, \infty)$. In Figure 3 we present an illustration of a node free state. Using (9a)–(9b) and following the same argument as in one–dimensional case, we can obtain the corresponding relation for two comparison potentials V_a and V_b

$$(E_b - E_a) \int_0^\infty (\psi_{1a}\psi_{1b} + \psi_{2a}\psi_{2b})dr = \int_0^\infty (V_b - V_a)(\psi_{1a}\psi_{1b} + \psi_{2a}\psi_{2b})dr. \tag{11}$$

From equation (11) we can eventually recover the basic comparison theorem [1] to the effect that if the radial components of the Dirac spinor are node free and $V_a \leq V_b$, then $E_a \leq E_b$.
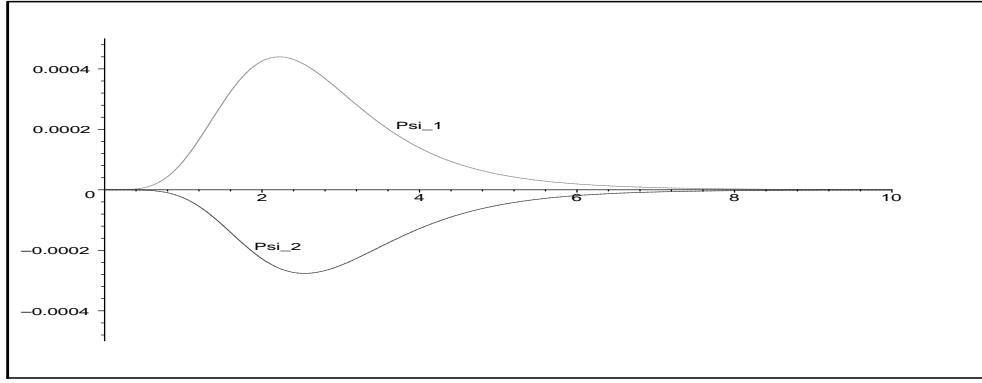
FIG. 3: The Dirac radial wave functions ψ_1 and ψ_2 at the bottom of an angular–momentum subspace labelled by j, corresponding to the Woods–Saxon potential [38] in the form $V = -\dfrac{v}{1 + e^{\frac{r-R}{a}}}$, with $v = 4$, $R = 2$, $a = 1.2$, $\tau = -1$, $d = 8$, $j = 3/2$, $m = 1$, and the energy eigenvalue is $E = 0.62317$.

A. Bounded Potentials

Here we suppose that the potential V in the Dirac equations (9a)–(9b) is such that

(i) V is nonpositive and bounded, i.e. $V_0 \leq V \leq 0$, where $V_0 = V(0)$;

(ii) V vanishes at infinity, thus $\lim\limits_{r \to \infty} V = 0$;

(iii) V is attractive, that is monotone nondecreasing on $[0, \infty)$; thus, when V is differentiable, $V' \geq 0$.

We shall first prove the following lemma, which characterizes the behaviour of the Dirac radial wave functions at the bottom of the angular–momentum subspace labelled by j: for these nodefree states [20], $k_d = -\left(j + \dfrac{d-2}{2}\right)$, where $j = 1/2,\ 3/2,\ 5/2,\ \ldots$ and $d = 2,\ 3,\ 4,\ \ldots$.

Lemma 1:   *the Dirac radial spinor components ψ_1 and ψ_2 at the bottom of an angular–momentum subspace labelled by j, which satisfy (9a)–(9b), for the bounded potential V are such that*

$$\left(\frac{\psi_1}{r^{|k_d|}}\right)' \leq 0 \quad and \quad \left(\frac{\psi_2}{r^{|k_d|+1}}\right)' \geq 0, \quad r \in [0,\ \infty).$$

Proof: Near the origin the system (9a)–(9b) may be rewritten as:

$$\begin{cases} \psi_1'' = \psi_1 \left(\dfrac{k_d(k_d+1)}{r^2} + m^2 - (E - V_0)^2\right), & \text{(12a)} \\[2mm] \psi_2'' = \psi_2 \left(\dfrac{k_d(k_d-1)}{r^2} + m^2 - (E - V_0)^2\right). & \text{(12b)} \end{cases}$$

Solutions of these equations involve Bessel functions. Hence for small r we can approximate them by simple powers in the following form

$$\begin{cases} \psi_1 = c_1 r^{q_1}, & \text{(13a)} \\ \psi_2 = c_2 r^{q_2}, & \text{(13b)} \end{cases}$$

where c_1 and c_2 are constants of integration and parameters q_1 and q_2 are positive since both wave functions must vanish at the origin. After substituting (13a)–(13b) into (9a)–(9b) and dividing one equation by the other we obtain the following relation

$$(q_1 + k_d)(q_2 - k_d) = (m + E - V_0)(m - E + V_0)r^2,$$

which in the limit as r approaches 0 reduces to

$$(q_1 + k_d)(q_2 - k_d) = 0.$$

Since $k_d < 0$ and $q_1 > 0$, it follows from the above expression that $q_1 = -k_d$. Then equation (9b) becomes:

$$c_2(q_2 - k_d)r^{q_2-1} = c_1(m - E + V_0)r^{-k_d}.$$

Equating the powers of r we obtain $q_2 = 1 - k_d$. Also one finds

$$\frac{c_1}{c_2} = \frac{1 - 2k_d}{m - E + V_0}.$$

According to (ii) and (iii), $\lim\limits_{r\to\infty}(m - E + V) = m - E > 0$, meanwhile $m - E + V_0 < 0$, thus the quantity $m - E + V$ changes sign exactly once [20] for $r > 0$. The ratio $c_1/c_2 < 0$, which means that ψ_1 and ψ_2 have opposite signs (this is in agreement with our assumption for the nodeless state, that is $\psi_1 \geq 0$ and $\psi_2 \leq 0$ on $[0, \infty)$). Finally, we conclude that near the origin radial wave functions behave as

$$\begin{cases} \psi_1 = C_1 r^{-k_d}, & \text{(14a)} \\ \psi_2 = C_2 r^{-k_d+1}. & \text{(14b)} \end{cases}$$

Now let us make the following substitution $\psi_1 = r^{-k_d}R_1$ and $\psi_2 = r^{-k_d+1}R_2$, then the system of equations (9a)–(9b) becomes

$$\begin{cases} R_1' = (m + E - V)rR_2, & \text{(15a)} \\ R_2' = (m - E + V)\dfrac{R_1}{r} + \dfrac{2k_d - 1}{r}R_2. & \text{(15b)} \end{cases}$$

According to (i) and (15a), $R_1' \leq 0$ which is equivalent to the lemma's first inequality. Since $m - E + V$ has to change sign from negative to positive, thus for large r, according to (15b), $R_2' \geq 0$. In order to determine the behaviour of the R_2' near the origin, we expand R_1 and R_2 in power series, i. e. $R_1 = a_0 + a_1 r + a_2 r^2 + a_3 r^3 + \ldots$ and $R_2 = b_0 + b_1 r + b_2 r^2 + b_3 r^3 + \ldots$, then system (15a)–(15b) implies

$$\begin{cases} R_1 = a_0 + a_2 r^2 + \ldots, & \text{(16a)} \\ R_2 = b_0 + b_2 r^2 + \ldots, & \text{(16b)} \end{cases}$$

where if $a_0 > 0$, then $b_0 < 0$, $a_2 < 0$, and $b_2 > 0$. Thus $R_2' \geq 0$ near zero.

Let us suppose that the function R_2 is decreasing on some interval $(r_1,\ r_2)$, i. e. $R_2' < 0$ on $(r_1,\ r_2)$ and $R_2'(r_1) = R_2'(r_2) = 0$. Then it follows from the Rolle's Theorem that there is at least one number $r_c \in (r_1,\ r_2)$ such that $R_2''(r_c) = 0$, which is equivalent to

$$\left((m - E + V)\frac{R_1}{r} + \frac{2k_d - 1}{r}R_2\right)' = 0 \quad \text{at} \quad r = r_c$$

or, using (15b),

$$V'R_1 + (m - E + V)R_1' + (2k_d - 2)R_2' = 0 \quad \text{at} \quad r = r_c.$$

In the above expression first two terms are nonnegative and $(2k_d - 2)R_2'$ is strictly positive, which yields a contradiction. Hence $R_2' \geq 0$ on $r \in [0,\ \infty)$ and this corresponds to the lemma's second inequality.

$\square$

Theorem 3: *The potential V, satisfies (i)–(ii), $V_0 \geq -2m$, and has $r^{2|k_d|}$-weighted area, if*

$$\eta(r) = \int_0^r (V_b(t) - V_a(t))t^{2|k_d|}dt \geq 0, \quad r \in [0,\ \infty), \tag{17}$$

then we have $E_a \leq E_b$.

Proof: Let us integrate the right side of (11) by parts in the following way

$$\int_0^\infty (V_b - V_a)(\psi_{1a}\psi_{1b} + \psi_{2a}\psi_{2b})dr = (\psi_{1a}\psi_{1b} + \psi_{2a}\psi_{2b})\frac{\eta}{r^{2|k_d|}}\Big|_0^\infty - \int_0^\infty \eta\left(\frac{\psi_{1a}\psi_{1b} + \psi_{2a}\psi_{2b}}{r^{2|k_d|}}\right)' dr,$$

where $\eta(r)$ is defined by (17). Since $\eta(0) = 0$ and $\lim_{r\to\infty} \psi_1 = \lim_{r\to\infty} \psi_2 = 0$ with the respective asymptotic forms (14a)–(14b), relation (11) becomes

$$(E_b - E_a) \int_0^\infty (\psi_{1a}\psi_{1b} + \psi_{2a}\psi_{2b})dr = -\int_0^\infty \eta \left(\frac{\psi_{1a}\psi_{1b} + \psi_{2a}\psi_{2b}}{r^{2|k_d|}} \right)' dr. \tag{18}$$

Using (9a)–(9b) we find

$$\left(\frac{\psi_{1a}\psi_{1b} + \psi_{2a}\psi_{2b}}{r^{2|k_d|}} \right)' = W_1 \frac{\psi_{1b}\psi_{2a}}{r^{2|k_d|}} + W_2 \frac{\psi_{1a}\psi_{2b}}{r^{2|k_d|}} + 4k_d \frac{\psi_{2a}\psi_{2b}}{r^{2|k_d|+1}},$$

where

$$W_1 = 2m + E_a - E_b - V_a + V_b \quad \text{and} \quad W_2 = 2m - E_a + E_b + V_a - V_b.$$

We know that quantity $m - E + V$ changes sign from negative to positive. When $m - E + V \leq 0$ we have $W_1 \geq 3m - E_b + V_b$. Since $-m < E < m$ and $V \geq -2m$, then $W_1 \geq 3m - E_b + V_b > 0$. When $m - E + V > 0$ it is straightforward that $W_1 \geq m + E_a - V_a > 0$. Therefore $W_1 > 0$ for $r \in [0, \infty)$. Similarly it can be shown that $W_2 > 0$. Thus the derivative $\left(\frac{\psi_{1a}\psi_{1b} + \psi_{2a}\psi_{2b}}{r^{2|k_d|}} \right)' \leq 0$ and according to the theorem's assumption (17) and equation (18) we have $E_a \leq E_b$.

$\square$

We note that above theorem, as well as Theorem 1, does not require a nondecreasing potential V on $[0, \infty)$, i. e. V can decrease on some intervals. As in the one–dimensional case, if we know more precise behaviour of the comparison potentials, we can state simpler sufficient conditions:

Corollary 3: *If the potentials cross over once, say at r_1, and $V_a \leq V_b$ for $r \in [0, \ r_1]$, and*

$$\eta(\infty) = \int_0^\infty (V_b - V_a)r^{2|k_d|}dr \geq 0,$$

then $E_a \leq E_b$. If the potentials cross over twice, say at r_1 and r_2, $r_1 < r_2$, $V_a \leq V_b$ for $r \in [0, \ r_1]$, and

$$\eta(r_2) = \int_0^{r_2} (V_b - V_a)r^{2|k_d|}dr \geq 0,$$

then $E_a \leq E_b$.

We can extend the above corollary in the following way: assume that comparison potentials have n intersections, $n = 1, 2, 3, \ldots$, and $V_a \leq V_b$ on $r \in [0, \ r_1]$. Also assume that $\int_{r_i}^{r_{i+1}} |V_b - V_a| r^{2|k_d|}dr$, $i = 1, 2, 3, \ldots, n$ is nonincreasing sequence (if n is odd then $\int_{r_{n-1}}^{r_n} |V_b - V_a| r^{2|k_d|}dr \geq \int_{r_n}^\infty |V_b - V_a| r^{2|k_d|}dr$), hence $\int_0^r (V_b(t) - V_a(t))t^{2|k_d|}dt \geq 0$, $r \in [0, \infty)$, and we conclude $E_a \leq E_b$.

Theorem 4: *The potential V satisfies (i)–(iii), and has $\psi_{1i}r^{|k_d|}$ and $\psi_{2i}r^{|k_d|+1}$–weighted areas, if*

$$\lambda_1(r) = \int_0^r (V_b(t) - V_a(t))\psi_{1i}(t)t^{|k_d|}dt \geq 0 \quad \text{and} \quad \lambda_2(r) = \int_0^r (V_b(t) - V_a(t))(-\psi_{2i}(t))t^{|k_d|+1}dt \geq 0, \tag{19}$$

$r \in [0, \infty)$, where i is either a or b, then we have $E_a \leq E_b$.

Proof: We prove the theorem for $i = b$; for $i = a$, the proof is the same. After integrating the right side of (11) by parts we obtain

$$\int_0^\infty (V_b - V_a)(\psi_{1a}\psi_{1b} + \psi_{2a}\psi_{2b})dr = \left[\lambda_1 \frac{\psi_{1a}}{r^{|k_d|}} + \lambda_2 \frac{\psi_{2a}}{r^{|k_d|+1}} \right]_0^\infty - \int_0^\infty \left[\lambda_1 \left(\frac{\psi_{1a}}{r^{|k_d|}} \right)' + \lambda_2 \left(\frac{\psi_{2a}}{r^{|k_d|+1}} \right)' \right] dr,$$

where $\lambda_1(r)$ and $\lambda_2(r)$ are defined by (19) for $i = b$. Since $\lambda_1(0) = \lambda_2(0) = 0$ and $\lim_{r\to\infty} \psi_{1a} = \lim_{r\to\infty} \psi_{2a} = 0$ with the respective asymptotic forms (14a)–(14b), expression (11) becomes

$$(E_b - E_a) \int_0^\infty (\psi_{1a}\psi_{1b} + \psi_{2a}\psi_{2b})dr = -\int_0^\infty \left[\lambda_1 \left(\frac{\psi_{1a}}{r^{|k_d|}} \right)' + \lambda_2 \left(\frac{\psi_{2a}}{r^{|k_d|+1}} \right)' \right] dr.$$
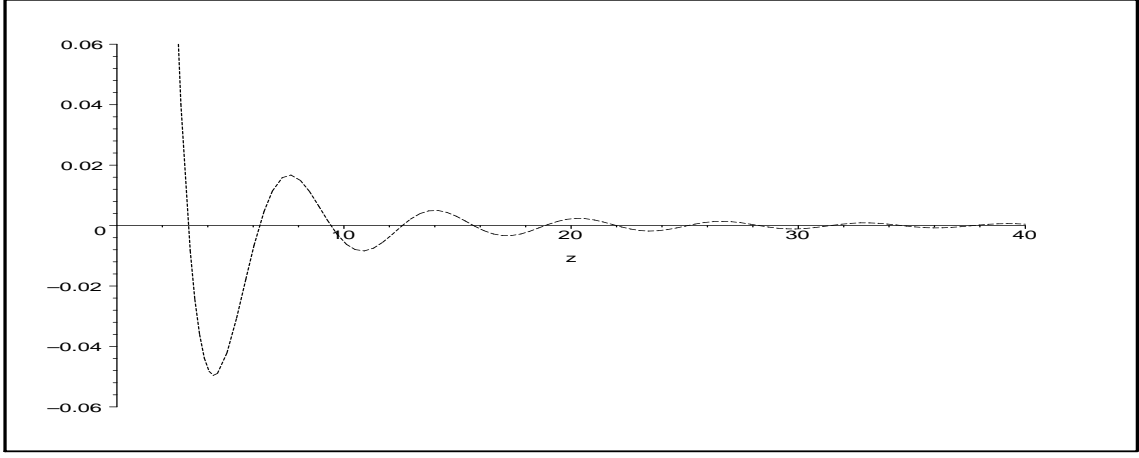
FIG. 4: The graph of the integrand $I = \dfrac{\sin z}{z^2}$.

Then Lemma 1 and the theorem's assumptions ensure that $E_a \leq E_b$.

□

Corollary 4:   *If the potentials cross over once, say at r_1, $V_a \leq V_b$ for $r \in [0, \ r_1]$, and*

$$\lambda_1(\infty) = \int_0^\infty (V_b - V_a)\psi_{1i}r^{|k_d|}dr \geq 0 \quad and \quad \lambda_2(\infty) = \int_0^\infty (V_b - V_a)(-\psi_{2i})r^{|k_d|+1}dr \geq 0, \quad i = a \ or \ b,$$

then $E_a \leq E_b$. If the potentials cross over twice, say at r_1 and r_2, $r_1 < r_2$, $V_a \leq V_b$ for $r \in [0, \ r_1]$, and

$$\lambda_1(r_2) = \int_0^{r_2} (V_b - V_a)\psi_{1i}r^{|k_d|}dr \geq 0 \quad and \quad \lambda_2(r_2) = \int_0^{r_2} (V_b - V_a)(-\psi_{2i})r^{|k_d|+1}dr \geq 0, \quad i = a \ or \ b,$$

then $E_a \leq E_b$.

As before we can generalize Corollary 4 to allow n intersections, i.e. if $V_a \leq V_b$ on $r \in [0, \ r_1]$ and both sequences of absolute areas $\int_{r_i}^{r_{i+1}} |(V_b - V_a)\psi_{1i}r^{|k_d|}|dr$ and $\int_{r_i}^{r_{i+1}} |(V_b - V_a)\psi_{2i}r^{|k_d|+1}|dr$, $i = a$ or b, are nonincreasing (if n is odd then we assume $\int_{r_{n-1}}^{r_n} |(V_b - V_a)\psi_{1i}r^{|k_d|}|dr \geq \int_{r_n}^{\infty} |(V_b - V_a)\psi_{1i}r^{|k_d|}|dr$ and $\int_{r_{n-1}}^{r_n} |(V_b - V_a)\psi_{2i}r^{|k_d|+1}|dr \geq \int_{r_n}^{\infty} |(V_b - V_a)\psi_{2i}r^{|k_d|+1}|dr)$, then integrals $\int_0^r (V_b(t) - V_a(t))\psi_{1i}(t)t^{|k_d|}dt \geq 0$ and $\int_0^r (V_b(t) - V_a(t))(-\psi_{2i}(t))t^{|k_d|+1}dt \geq 0$ for $r \in [0, \ \infty)$, thus $E_a \leq E_b$.

An example

As an example we consider Theorem 3, in particular Corollary 3 for the case of many intersections. We take the following comparison potentials

$$V_a = -\frac{\alpha}{ur^3 + a}\left(1 + \frac{v\sin(\kappa r^3 + s)}{\kappa r^3 + s}\right) \qquad \text{and} \qquad V_b = -\frac{\beta}{wr^3 + b}.$$

If $\alpha = \beta$, $a = s = b$, $u = \kappa = w$, $\tau = -1$, $j = 1/2$, and $d = 3$ the substitution $z = ur^3 + a$ transforms the integral (17) into

$$\int_0^\infty (V_b - V_a)r^2 dt = \frac{\alpha v}{3u}\int_a^\infty \frac{\sin z}{z^2}dz.$$

The integrand $I = \dfrac{\sin z}{z^2}$ is plotted on Figure 4. Choosing $a = 2.04$, and calculating numerical values, we find that the first area is bigger then the second one:

$$\int_a^\pi \frac{|\sin z|}{z^2}dz = 0.0965 > \int_\pi^{2\pi} \frac{|\sin z|}{z^2}dz = 0.0962.$$

The $\sin z$ is the periodic function, thus $|\sin x| = |\sin y|$ where $x \in [(k-1)\pi,\ k\pi]$ and $y = x + \pi$, $k = 3,\ 4,\ 5,\ \ldots$, then it is clear that

$$\int_{(k-1)\pi}^{k\pi} \frac{|\sin z|}{z^2} dz > \int_{k\pi}^{(k+1)\pi} \frac{|\sin z|}{z^2} dz.$$

Therefore

$$\int_0^\infty (V_b - V_a) r^2 dt \geq 0,$$

because successive positive and negative areas of the integrand do not increase in absolute value. Thus $\eta > 0$ and by Theorem 3 we have $E_a \leq E_b$. This prediction is verified by accurate numerical calculations: for $\alpha = 3.4$, $a = 2.04$, $v = 0.4$, and $u = 7$ the comparison potentials intersect at infinitely many points (see Figure 5), with $m = 1$ so that condition $-2m \leq V_0$ is satisfied. Accurate numerical eigenvalues are $E_a = 0.99427 \leq E_b = 0.99542$.
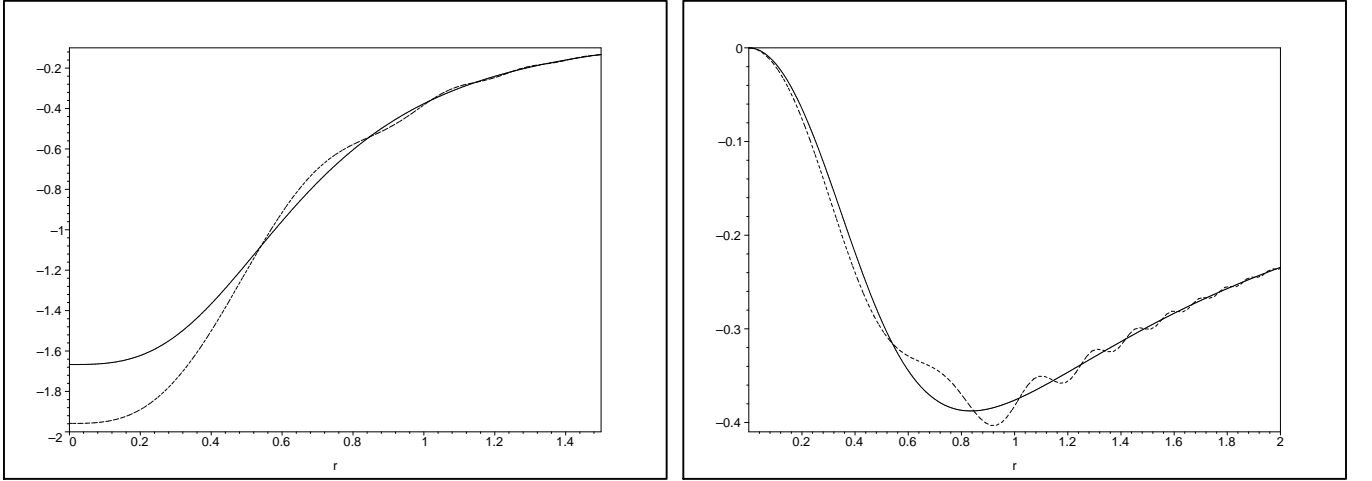

FIG. 5: Left graph: potential V_a dashed line and V_b full line. Right graph: function $V_a r^{2|k_d|}$ dashed line and $V_b r^{2|k_d|}$ full line.

B. Unbounded Potentials

We consider a class of unbounded potentials of the form $V(r) = -\dfrac{f(r)}{r}$, where the bounded factor f satisfies:

(iv) f is nonnegative and bounded, i.e. $f_0 \geq f \geq 0$, where $f_0 = \lim_{r \to 0^+} f$;

(v) f is monotone nonincreasing on $[0, \infty)$, so $f' \leq 0$;

(vi) V vanishes at infinity, so $\lim_{r \to \infty} \dfrac{f}{r} = 0$.

For instance, for the Coulomb potential $V = -\dfrac{v}{r}$, the function $f = v$, for the Yukawa potential [39] $V = -\dfrac{v}{re^{\lambda r}}$, the function $f = \dfrac{v}{e^{\lambda r}}$, for the Hulthén potential [40] $V = -\dfrac{v}{e^{\lambda r} - 1}$, the function $f = \dfrac{vr}{e^{\lambda r} - 1}$, and so on.

Lemma 2: *the Dirac radial spinor components ψ_1 and ψ_2 at the bottom of an angular–momentum subspace labelled by j, which satisfy (9a)–(9b), for the potential $V = -\dfrac{f}{r}$ are such that*

$$\left(\frac{\psi_1}{r^{|k_d|}} \right)' \leq 0 \quad and \quad \left(\frac{\psi_2}{r^{|k_d|}} \right)' \geq 0, \quad r \in [0,\ \infty).$$

Proof: For small r analysis of the Dirac coupled equations (9a)–(9b) yields the asymptotic forms:

$$\begin{cases} \psi_1'' = \psi_1 \dfrac{k_d^2 - f_0^2}{r^2} - \dfrac{\psi_1'}{r}, & \text{(20a)} \\[3mm] \psi_2'' = \psi_2 \dfrac{k_d^2 - f_0^2}{r^2} - \dfrac{\psi_2'}{r}. & \text{(20b)} \end{cases}$$

These are Cauchy-Euler equations with solution in the form [41]:

$$\begin{cases} \psi_1 = c_1 r^\gamma, & \text{(21a)} \\[2mm] \psi_2 = c_2 r^\gamma, & \text{(21b)} \end{cases}$$

where c_1 and c_2 are constants of integration, and the parameter γ has to be positive because the wave functions must vanish at the origin. Substitution of (21a)–(21b) into (9a)–(9b) yields

$$\begin{cases} \gamma = f_0 c_2/c_1 - k_d, \\[2mm] \gamma = -f_0 c_1/c_2 + k_d. \end{cases}$$

The solution of the above system is: $\gamma = \sqrt{k_d^2 - f_0^2}$ and $\dfrac{c_2}{c_1} = \dfrac{k_d \pm \sqrt{k_d^2 - f_0^2}}{f_0}$. As in sec. A, $c_2/c_1 < 0$, which is in agreement with our assumption for the nodeless state. Therefore near 0 the wave functions behave as

$$\begin{cases} \psi_1 = c_1 r^{\sqrt{k_d^2 - f_0^2}}, \\[2mm] \psi_2 = c_2 r^{\sqrt{k_d^2 - f_0^2}}. \end{cases}$$

We now substitute $\psi_1 = r^{-k_d} P_1$ and $\psi_2 = r^{-k_d} P_2$, into (9a)–(9b) to obtain:

$$\begin{cases} P_1' = (m + E - V)P_2, & \text{(24a)} \\[3mm] P_2' = (m - E + V)P_1 + \dfrac{2k_d}{r} P_2. & \text{(24b)} \end{cases}$$

Clearly, $P_1' \leq 0$ which is equivalent to the lemma's third inequality. Near the origin P_2 behaves as $c_2 r^{\sqrt{k_d^2 - f_0^2} + k_d}$, thus $P_2' \geq 0$ near 0. At infinity (24b) becomes $P_2' = (m - E)P_1$, so $P_2' \geq 0$ near infinity. Let us assume that $P_2' < 0$ on some (r_1, r_2), so $P_2(r_1) = P_2(r_2) = 0$. Then by Rolle Theorem, there exists r_c such that $P_2''(r_c) = 0$, which corresponds to

$$(m - E + V)P_1' + \left(V' + \frac{V}{r}\right)P_1 + (2k_d - 1)\frac{P_2'}{r} + (m - E)\frac{P_1}{r} = 0 \quad \text{at} \quad r = r_c.$$

Since $V = -\dfrac{f}{r}$, the expression $V' + \dfrac{V}{r} = -\dfrac{f'}{r}$ is nonnegative according to (v). Therefore in the above expression the first two terms are nonnegative and the last two are strictly positive, which observation reveals a contradiction. Therefore $P_2' \geq 0$ on $r \in [0, \infty)$ and this is equivlent to the lemma's last inequality.

$\square$

Now we state and prove the refined comparison theorem for a special class of unbounded potentials:

Theorem 5: *The potential* $V = -\dfrac{f}{r}$, *where* f *satisfies* (iv)–(vi), *has* $\psi_{1i} r^{|k_d|}$ *and* $\psi_{2i} r^{|k_d|}$*–weighted areas, if*

$$\rho_1(r) = \int_0^r (V_b(t) - V_a(t))\psi_{1i}(t) t^{|k_d|} dt \geq 0 \quad and \quad \rho_2(r) = \int_0^r (V_b(t) - V_a(t))(-\psi_{2i}(t)) t^{|k_d|} dt \geq 0, \qquad \text{(25)}$$

$r \in [0, \infty)$, *where* i *is either* a *or* b, *then we have* $E_a \leq E_b$.

Proof: We prove the theorem for $i = a$; for $i = b$, the proof is the same. As in sec. A we integrate the right side of (11) by parts to obtain

$$\int_0^\infty (V_b - V_a)(\psi_{1a}\psi_{1b} + \psi_{2a}\psi_{2b})dr = -\int_0^\infty \left[\eta_1 \left(\frac{\psi_{1a}}{r^{|k_d|}}\right)' + \eta_2 \left(\frac{\psi_{2a}}{r^{|k_d|}}\right)'\right] dr,$$

where $\eta_1(r)$ and $\eta_2(r)$ are defined by (25) for $i = a$. Then it follows from last two inequalities of the Lemma 2 and (25) that $E_a \leq E_b$.

$\square$

Corollary 5: *If the potentials cross over once, say at r_1, $V_a \leq V_b$ for $r \in [0,\ r_1]$, and*

$$\rho_1(\infty) = \int_0^\infty (V_b - V_a)\psi_{1i}r^{|k_d|}dr \geq 0 \quad and \quad \rho_2(\infty) = \int_0^\infty (V_b - V_a)(-\psi_{2i})r^{|k_d|}dr \geq 0, \quad i = a \text{ or } b,$$

then $E_a \leq E_b$. If the potentials cross over twice, say at r_1 and r_2, $r_1 < r_2$, $V_a \leq V_b$ for $r \in [0,\ r_1]$, and

$$\rho_1(r_2) = \int_0^{r_2} (V_b - V_a)\psi_{1i}r^{|k_d|}dr \geq 0 \quad and \quad \rho_2(r_2) = \int_0^{r_2} (V_b - V_a)(-\psi_{2i})r^{|k_d|}dr \geq 0, \quad i = a \text{ or } b,$$

then $E_a \leq E_b$.

The above Corollary can be generalized up to n intersections: if $V_a \leq V_b$ on $r \in [0,\ r_1]$ and both sequences of absolute areas $\int_{r_i}^{r_{i+1}} |(V_b - V_a)\psi_{1i}r^{|k_d|}|dr$ and $\int_{r_i}^{r_{i+1}} |(V_b - V_a)\psi_{2i}r^{|k_d|}|dr$, $i = a$ or b, are nonincreasing (if n is odd then we assume $\int_{r_{n-1}}^{r_n} |(V_b - V_a)\psi_{1i}r^{|k_d|}|dr \geq \int_{r_n}^{\infty} |(V_b - V_a)\psi_{1i}r^{|k_d|}|dr$ and $\int_{r_{n-1}}^{r_n} |(V_b - V_a)\psi_{2i}r^{|k_d|}|dr \geq \int_{r_n}^{\infty} |(V_b - V_a)\psi_{2i}r^{|k_d|}|dr$), then $\eta_1(r) \geq 0$ and $\eta_2(r) \geq 0$ for $r \in [0,\ \infty)$, thus $E_a \leq E_b$.

<center>*An example*</center>

Here we will demonstrate first part of Corollary 5, i. e. the case of one intersection. For the comparison potentials we choose the Hulthén potential V_a and the Coulomb potential V_b:

$$V_a = -\frac{\alpha}{e^{ar} - 1} \quad \text{and} \quad V_b = -\frac{\beta}{r}.$$

The above potentials intersect at exactly one point for $\alpha = 1/5$, $a = 3/10$, and $\beta = 0.508$; Figure 6, left graph. We can see that $V_a \leq V_b$ before the intersection point. If $\rho_1(\infty)$ and $\rho_2(\infty)$ are both nonnegative, according to Corollary 5, we have $E_a \leq E_b$.

The solutions of the Dirac Coulomb problem are well known. In three dimensional ground state for $j = 1/2$, $\tau = -1$, and $m = 2$ the eigenvalue is [6]

$$E_b = 2\gamma$$

and the wave functions are

$$\left.\begin{array}{c}\psi_{1b}\\\psi_{2b}\end{array}\right\} = \pm\sqrt{\frac{2\beta(1 \pm \gamma)}{\Gamma(2\gamma + 1)}\frac{(4\beta r)^\gamma}{e^{2\beta r}}},$$

where $\gamma = \sqrt{1 - \beta^2}$, and Γ is the gamma function (the wave functions are plotted on Figure 6, right graph). Then $\rho_1(\infty) = 0.00113$ and $\rho_2(\infty) = 0.00031$ and, according to accurate numerical calculation, $E_a = 1.58604 \leq E_b = 1.72271$.

<center>**C.   Potentials less singular than Coulomb.**</center>

We characterize this class of potentials in the following way:

> *(vii)* V is nonpositive and unbounded, i.e. $V \leq 0$ and $\lim_{r\to 0^+} V = -\infty$;
>
> *(viii)* V is attractive, that is monotone nondecreasing on $[0, \infty)$ so $V' \geq 0$;
>
> *(ix)* V vanishes at infinity, thus $\lim_{r\to\infty} V = 0$;
>
> *(x)* V is less singular than Coulomb potential, i.e. $\lim_{r\to 0^+} rV = 0$.

Examples of such potentials are: $V = -\dfrac{v}{r^q}$, $V = -\dfrac{v}{r^q + r^b}$, and $V = -\dfrac{v}{r^q e^{br}}$, where $q \in (0,\ 1)$, v and b are positive constants. Then, as before, we first prove a lemma, namely
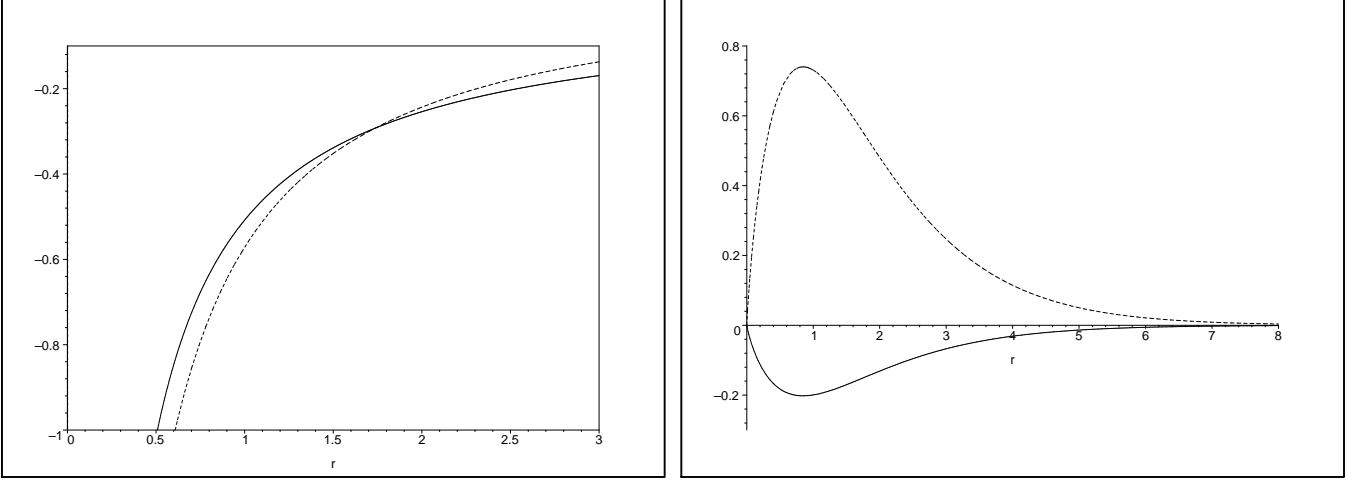
FIG. 6: Left graph: The Hulthén potential V_a dotted line and the Coulomb potential V_b full line. Right graph: Upper component of the Dirac spinor ψ_{1b} dotted line and lower component ψ_{2b} full line.
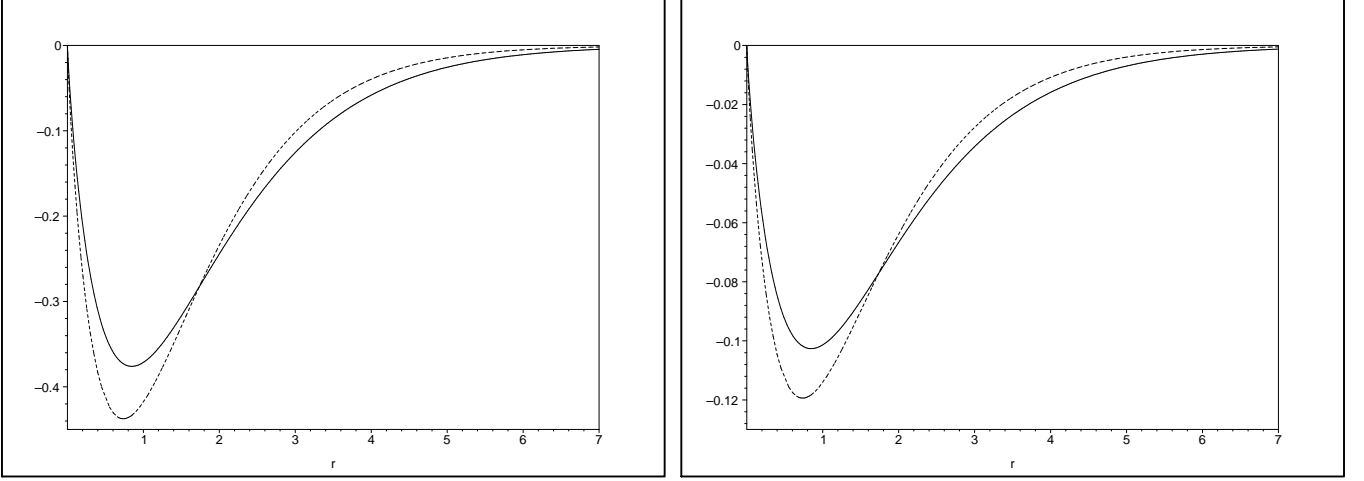

FIG. 7: Left graph: Function $V_a\psi_{1b}r$ dotted line and $V_b\psi_{1b}r$ full line. Right graph: Function $V_a(-\psi_{2b})r$ dotted line and $V_b(-\psi_{2b})r$ full line.

Lemma 3: *the Dirac radial spinor components ψ_1 and ψ_2 at the bottom of an angular–momentum subspace labelled by j, which satisfy (9a)–(9b), for the potential V, which satisfies (i)–(iv), are such that*

$$\left(\frac{\psi_1}{r^{|k_d|}}\right)' \leq 0 \quad and \quad \left(\frac{\psi_2}{r^{|k_d|+1}}\right)' \geq 0, \quad r \in [0, \infty).$$

Proof: Near the origin the above class of the potentials can be approximated by $V = -\dfrac{v}{r^q}$, then the system (9a)–(9b) after some rearrangements becomes:

$$\begin{cases} \psi_1'' = \psi_1 \left(\dfrac{k_d(k_d+1-q)}{r^2} - \dfrac{v^2}{r^{2q}}\right) - \psi_1'\dfrac{q}{r}, & \text{(26a)} \\[3mm] \psi_2'' = \psi_2 \left(\dfrac{k_d(k_d-1+q)}{r^2} - \dfrac{v^2}{r^{2q}}\right) - \psi_2'\dfrac{q}{r}. & \text{(26b)} \end{cases}$$
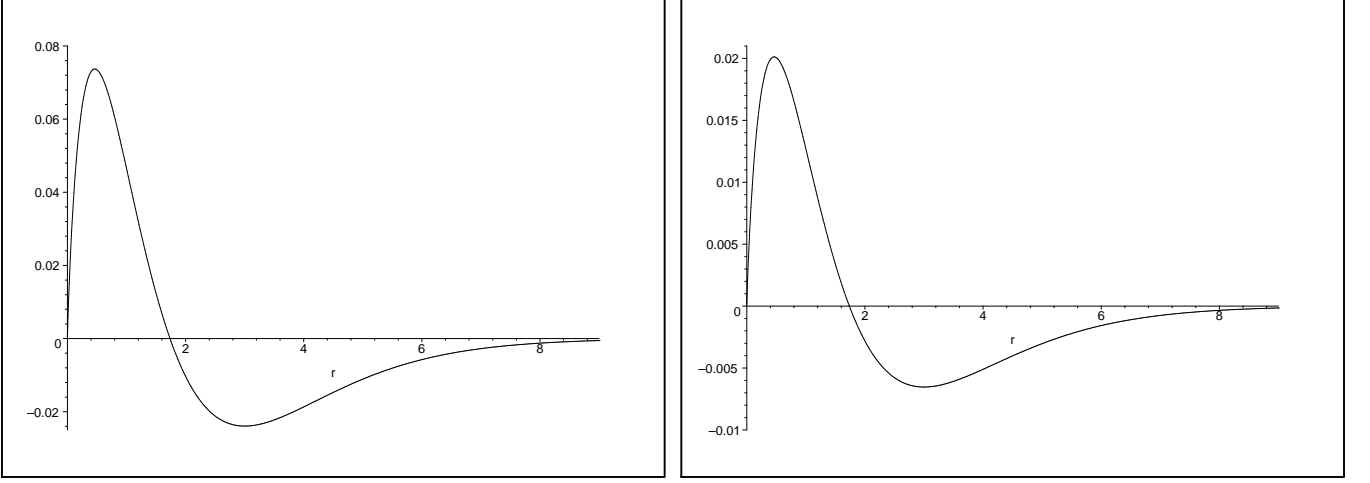
FIG. 8: Left graph: The graph of the integrand $(V_b - V_a)\psi_{1b}r$. Right graph: The graph of the integrand $(V_b - V_a)(-\psi_{2b})r$.

Solutions of these equations are given in terms of Bessel functions. Therefore for small r we can approximate them by simple powers

$$\begin{cases} \psi_1 = c_1 r^{q_1}, & \text{(27a)} \\ \psi_2 = c_2 r^{q_2}, & \text{(27b)} \end{cases}$$

where c_1 and c_2 are constants of integration and parameters q_1 and q_2 are positive since both wave functions must vanish at the origin. Then, following the proof of Lemma 1, we find $q_1 = -k_d$, $q_2 = -k_d - q + 1$, and $\dfrac{c_1}{c_2} = -\dfrac{1 - q - 2k_d}{v} < 0$. Thus, near the origin radial wave functions behave as

$$\begin{cases} \psi_1 = c_1 r^{-k_d}, \\ \psi_2 = c_2 r^{-k_d - q + 1}. \end{cases}$$

Now let us make the following substitution $\psi_1 = r^{-k_d} R_1$ and $\psi_2 = r^{-k_d + 1} R_2$, then the system of equations (9a)–(9b) becomes

$$\begin{cases} R_1' = (m + E - V) r R_2, & \text{(29a)} \\ R_2' = (m - E + V)\dfrac{R_1}{r} + \dfrac{2k_d - 1}{r} R_2. & \text{(29b)} \end{cases}$$

According to (vii) and (29a), $R_1' \leq 0$ which is equivalent to the lemma's first inequality. Near 0 the function R_2 behaves as $c_2 r^{-q}$, thus $R_2' \geq 0$ near 0. Equations (29a)–(29b) are exactly the same as (15a)–(15b), thus it can be proved by contradiction that $R_2' \geq 0$ on $r \in [0, \infty)$ which is the same as the lemma's second inequality.

$\square$

Since Lemma 1 and Lemma 3 have the same conclusions, the following theorem along with the corollary can be stated and proved as in the bounded case:

Theorem 6: *The potential V satisfies (vii)–(x), has $\psi_{1i} r^{|k_d|}$ and $\psi_{2i} r^{|k_d| + 1}$–weighted areas, if*

$$\mu_1(r) = \int_0^r (V_b(t) - V_a(t))\psi_{1i}(t) t^{|k_d|} dt \geq 0 \quad and \quad \mu_2(r) = \int_0^r (V_b(t) - V_a(t))(-\psi_{2i}(t)) t^{|k_d| + 1} dt \geq 0, \qquad \text{(30)}$$

$r \in [0, \infty)$, where i is either a or b, then we have $E_a \leq E_b$.

Corollary 6: *If the potentials cross over once, say at r_1, $V_a \leq V_b$ for $r \in [0, r_1]$, and*

$$\mu_1(\infty) = \int_0^\infty (V_b - V_a)\psi_{1i} r^{|k_d|} dr \geq 0 \quad and \quad \mu_2(\infty) = \int_0^\infty (V_b - V_a)(-\psi_{2i}) r^{|k_d| + 1} dr \geq 0, \quad i = a \text{ or } b,$$

then $E_a \leq E_b$. If the potentials cross over twice, say at r_1 and r_2, $r_1 < r_2$, $V_a \leq V_b$ for $r \in [0, r_1]$, and

$$\mu_1(r_2) = \int_0^{r_2} (V_b - V_a)\psi_{1i} r^{|k_d|} dr \geq 0 \quad and \quad \mu_2(r_2) = \int_0^{r_2} (V_b - V_a)(-\psi_{2i}) r^{|k_d|+1} dr \geq 0, \quad i = a \ or \ b,$$

then $E_a \leq E_b$.

As before Corollary 6 can be generalized to the case of n intersections.

D. General refined comparison theorem

In this section we shall construct the refined comparison theorem which combines all the above cases, i.e. bounded, unbounded, and less singular than Coulomb potentials. First, we state the following lemma:

Lemma 4: *the Dirac radial spinor components ψ_1 and ψ_2 at the bottom of an angular–momentum subspace labelled by j, which satisfy (9a)–(9b), for the bounded potential (satisfies (i)–(iii)), or for the unbounded potential (satisfies (iv)–(vi)), or for the potential less singular than Coulomb (satisfies (vii)–($\times$)) are such that*

$$\left(\frac{\psi_1}{r^{|k_d|}}\right)' \leq 0 \quad and \quad \left(\frac{\psi_2}{r^{|k_d|+1}}\right)' \geq 0, \quad r \in [0, \infty).$$

Proof: The proof for the bounded and less singular than Coulomb potentials follows from Lemma 1 and 3 respectively, so we have to prove the Lemma for the unbounded case only.

Let us consider equations (9a)–(9b) with substitution $\psi_1 = r^{-k_d}G_1$ and $\psi_2 = r^{-k_d+1}G_2$:

$$\begin{cases} G_1' = (m + E - V)rG_2, & \text{(31a)} \\ G_2' = (m - E + V)\dfrac{G_1}{r} + \dfrac{2k_d - 1}{r}G_2. & \text{(31b)} \end{cases}$$

Then the lemma's first inequality follows from (31a). We know from the proof of Lemma 2 that G_2 behaves near the origin as $c_2 r^{\sqrt{k_d^2 - f_0^2} + k_d - 1}$, where the constant $c_2 < 0$, therefore $G_2' \geq 0$ near 0. Since $(m - E + V) \geq 0$ near infinity, then according to (31b), function $G_2' \geq 0$ near infinity. Finally, it can be shown by contradiction that $G_2' \geq 0$ on $r \in [0, \infty)$, which ends the proof.

$\square$

Using the above Lemma, the general refined comparison theorem can be proved:

Theorem 7: *The potential V satisfies either (i)–(iii), or (iv)–(vi), or (vii)–($\times$), has $\psi_{1i} r^{|k_d|}$ and $\psi_{2i} r^{|k_d|+1}$–weighted areas, if*

$$\zeta_1(r) = \int_0^r (V_b(t) - V_a(t))\psi_{1i}(t)t^{|k_d|} dt \geq 0 \quad and \quad \zeta_2(r) = \int_0^r (V_b(t) - V_a(t))(-\psi_{2i}(t))t^{|k_d|+1} dt \geq 0, \quad \text{(32)}$$

$r \in [0, \infty)$, where i is either a or b, then we have $E_a \leq E_b$.

Corollary 7: *If the potentials cross over once, say at r_1, $V_a \leq V_b$ for $r \in [0, r_1]$, and*

$$\zeta_1(\infty) = \int_0^\infty (V_b - V_a)\psi_{1i} r^{|k_d|} dr \geq 0 \quad and \quad \zeta_2(\infty) = \int_0^\infty (V_b - V_a)(-\psi_{2i}) r^{|k_d|+1} dr \geq 0, \quad i = a \ or \ b,$$

then $E_a \leq E_b$. If the potentials cross over twice, say at r_1 and r_2, $r_1 < r_2$, $V_a \leq V_b$ for $r \in [0, r_1]$, and

$$\zeta_1(r_2) = \int_0^{r_2} (V_b - V_a)\psi_{1i} r^{|k_d|} dr \geq 0 \quad and \quad \zeta_2(r_2) = \int_0^{r_2} (V_b - V_a)(-\psi_{2i}) r^{|k_d|+1} dr \geq 0, \quad i = a \ or \ b,$$

then $E_a \leq E_b$.

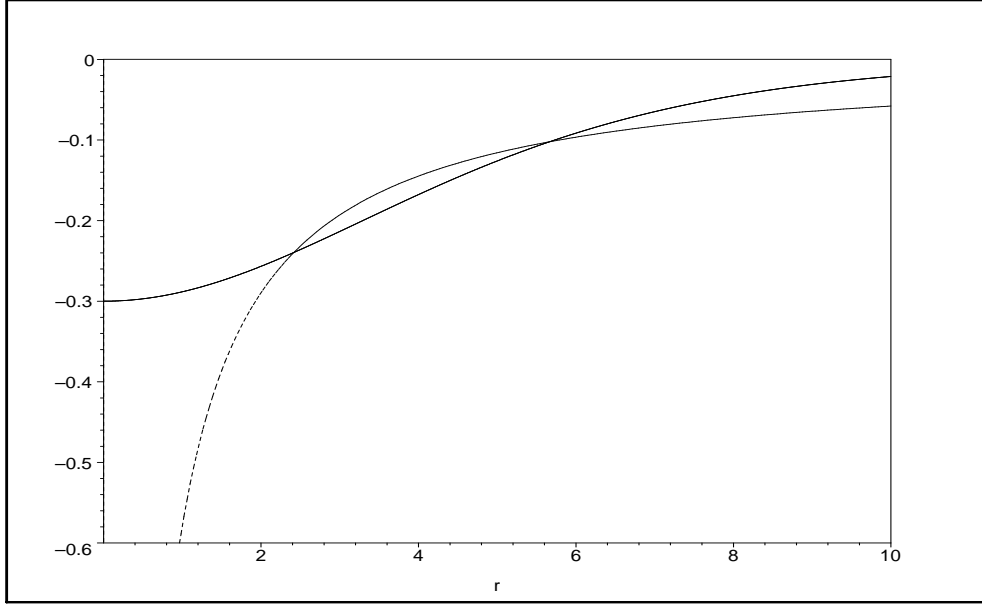As before Corollary 7 can be generalized to the case of n intersections.

FIG. 9: The Coulomb potential V_a dotted line and the Sech–squared potential V_b full line.

An example

In that section we will demonstrate the second part of Corollary 7, using unbounded Coulomb potential V_a and bounded Sech–squared potential V_b, which has been known under several different names since early days of quantum mechanics such as the Pöschl-Teller potential [42] or the Eckart potential [43]:

$$V_a = -\frac{\alpha}{r} \qquad \text{and} \qquad V_b = -\beta\text{sech}^2 br.$$

If $\alpha = 0.579$, $\beta = 0.3$, and $b = 0.2$ then V_a and V_a intersect at exactly two points $r_1 = 2.41742$ and $r_2 = 5.66301$; see Figure 9. According to [6], in $d = 3$ dimensions for $j = 1/2$, $\tau = -1$, and $m = 1$ the wave functions and the eigenvalue are:

$$\left.\begin{array}{c}\psi_{1a}\\\psi_{2a}\end{array}\right\} = \pm\sqrt{\frac{\alpha(1\pm\gamma)}{\Gamma(2\gamma+1)}}\frac{(2\alpha r)^\gamma}{e^{\alpha r}}, \qquad \text{and} \qquad E_a = \gamma,$$

where $\gamma = \sqrt{1-\alpha^2}$, and Γ is the gamma function. Then direct calculation shows that $\zeta_1(r_2) = 0.18778$ and $\zeta_2(r_2) = 0.00084$. Thus Corollary 7 implies that $E_a \leq E_b$, which agrees with the accurate numerical energy eigenvalies: $E_a = 0.81533 \leq E_b = 0.88318$.

VI. CONCLUSION

In this paper we have rederived the earlier comparison theorems in d dimensions and then refined these theorems by allowing the comparison potentials to crossover in a controlled manner. Because of the different form of the Dirac coupled equations in $d = 1$ and $d > 1$ dimensions we have studied these cases separately. We have shown that in one dimension the condition $V_a \leq V_b$, which leads to the spectral ordering $E_a \leq E_b$, can be replaced by weaker condition $U_a \leq U_b$, where $U_i(x) = \int_0^x V_i(t)dt$ $i = a$ or b. Since the potential cross–over conditions depend on the detailed behaviour of the radial wave–functions components, we have found it best in $d > 1$ dimensions to establish first a separate refined comparison theorem for each of a number of interesting classes of potential: Theorems 3 and 4 for bounded potentials, Theorem 5 for unbounded potentials, and Theorem 6 for the class of potentials less singular than Coulomb. Finally, we have summarized the refined comparison results in Theorem 7, which combines all of the above types of potentials and states that if $U_{1a} \leq U_{1b}$ and $U_{2a} \leq U_{2b}$ then $E_a \leq E_b$, where $U_{1i}(r) = \int_0^r V_i(t)\psi_{1j}(t)t^{|k_d|}dt$ and $U_{2i}(r) = \int_0^r V_i(t)(-\psi_{2j}(t))t^{|k_d|+1}dt$, where i, $j = a$ or b.
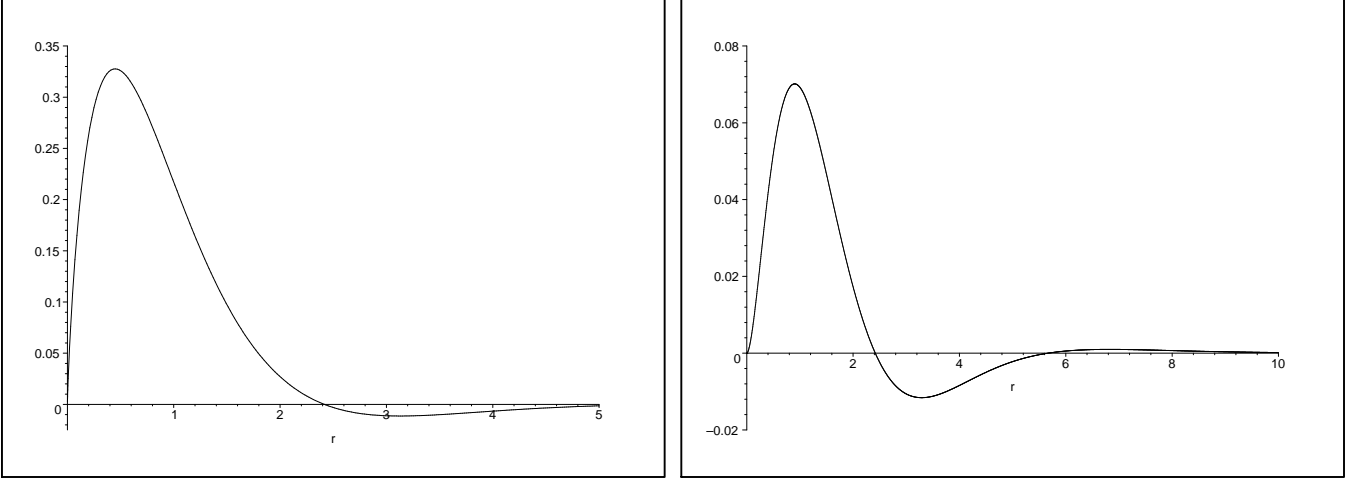
FIG. 10: Left graph: The graph of the integrand $(V_b - V_a)\psi_{1b}r$. Right graph: The graph of the integrand $(V_b - V_a)(-\psi_{2b})r^2$.

For practical reasons we have also established weaker sufficient conditions, as corollaries, which guarantee in simple ways that the comparison potentials crossover so as to imply definite spectral ordering. These results are illustrated by some specific examples.

VII.   ACKNOWLEDGMENTS

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